Effect of Sb Segregation on Conductance and Catalytic Activity at Pt/Sb-Doped SnO2 Interface: A Synergetic Computational and Experimental Study - DTU Orbit (08/11/2017)

Effect of Sb Segregation on Conductance and Catalytic Activity at Pt/Sb-Doped SnO_2 Interface: A Synergetic Computational and Experimental Study

Antimony doped tin dioxide (ATO) is considered a promising support material for Pt-based fuel cell cathodes, displaying enhanced stability over carbon-based supports. In this work, the effect of Sb segregation on the conductance and catalytic activity at Pt/ATO interface was investigated through a combined computational and experimental study. It was found that Sb-dopant atoms prefer to segregate toward the ATO/Pt interface. The deposited Pt catalysts, interestingly, not only promote Sb segregation, but also suppress the occurrence of Sb3+ species, a charge carrier neutralizer at the interface. The conductivity of ATO was found to increase, to a magnitude close to that of activated carbon, with an increment of Sb concentration before reaching a saturation point around 10%, and then decrease, indicating that Sb enrichment at the ATO surface may not always favor an increment of the electric current. In addition, the calculation results show that the presence of Sb dopants in ATO has little effect on the catalytic activity of deposited three-layer Pt toward the oxygen reduction reaction, although subsequent alloying of Pt and Sb could lower the corresponding catalytic activity. These findings help to support future applications of ATO/Pt-based materials as possible cathodes for PEMFC applications with enhanced durability under practical applications.

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